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A data assimilation system for specifying the thermospheric developed over the last several years. The particular benefit creation of a data assimilation system that makes use of a physical model, the Coupled Thermosphere-Ionosphere Model (CTIM) (Fuller-Rowell et al.,1996). The advantage of the physical model, CTIM, over empirical models comes from its ability to represent unclimatological features that are often present during geomagnetic storm conditions. A physical model, like CT1M, in a predictor/corrector-type data assimilation technique like the Kalnan filter, is ideal since the physical model has the ability to provide the 'best' state of the thermosphere based on conditions at a previous time. Correcting the physical model with observations, in a statistically rigorous manner, provides an optimal method for minimizing the errors while representing the time-dependent conditions of the thermospheric density. Because the thermosphere is strongly driven by external processes, the thrust of the research in the most recent years has focused primarily on improving the specification of the drivers. It has been shown that improved driver specification can greatly improve accuracy during geomagnetic storms. Improved driver specification has proven itself to be essential since satellite coverage is not globally available at a single epoch and since the upper atmosphere can change much more rapidly in comparison to the satellite revisit rate during geomagnetic storms.

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Abstract

A data assimilation system for specifying the thermospheric density has been developed over the last several years. The particular benefit of this research is the creation of a data assimilation system that makes use of a physical model, the Coupled Thermosphere-Ionosphere Model (CTIM) (Fuller-Rowell et al., 1996). The advantage of the physical model, CTIM, over empirical models comes from its ability to represent unclimatological features that are often present during geomagnetic storm conditions. A physical model, like CTIM, in a predictor/corrector-type data assimilation technique like the Kalman filter, is ideal since the physical model has the ability to provide the 'best' state of the thermosphere based on conditions at a previous time. Correcting the physical model with observations, in a statistically rigorous manner, provides an optimal method for minimizing the errors while representing the time-dependent conditions of the thermospheric density. Because the thermosphere is strongly driven by external processes, the thrust of the research in the most recent years has focused primarily on improving the specification of the drivers. It has been shown that improved driver specification can greatly improve accuracy during geomagnetic storms. Improved driver specification has proven itself to be essential since satellite coverage is not globally available at a single epoch and since the upper atmosphere can change much more rapidly in comparison to the satellite revisit rate during geomagnetic storms.

Overview

In the most recent years of this project, the main thrust has primarily focused on specifying the thermospheric drivers. In meteorological and ocean data assimilation, the fluid atmosphere or ocean is also described by a constantly changing state. In comparison to the troposphere, however, estimating the upper atmosphere brings about even greater challenges as the winds typically have higher speeds in the range of hundreds of meters per second. Additionally, the coverage is poorer for the upper atmosphere in comparison to the more numerous observation sources available to the meteorological and oceanographic communities. As a result, the state describing the neutral atmospheric density can change significantly between observations – particularly during geomagnetic storms.

Because the upper atmosphere is strongly forced, driver specification can also be used to one's advantage. Unlike the troposphere, external processes drive most of the variability in the upper atmospheric dynamics. During quiet times, the Sun directly heats the upper atmosphere by solar radiation in the extreme ultraviolet (EUV) frequencies. EUV heating occurs on the sunlit side of Earth with the maximum heating occurring at the region nearest to the sub-solar point. In the troposphere, for example, much of the variability arises from internal stochastic processes and is not strongly localized. Unlike the troposphere, most of the minute-to-minute variability in the thermosphere arises from the magnetospheric source imposed at high latitudes. During geomagnetic storm times, the heating process becomes more complicated and even more spatially and temporally variable. Geomagnetic storms occur when material, ejected from the sun by a coronal mass ejection, hits the Earth's magnetosphere. If the solar wind plasma has a southward magnetic field, it creates a coupling with the magnetosphere. Initially, plasma convection increases and auroral particle precipitation expands to lower latitudes. Besides the increased heating rate from particle precipitation and from Joule dissipation, the expanded convective electric field also redistributes the plasma.

As often occurs during geomagnetic storms, localized heating can result from the particle precipitation and Joule heating. Localized heating creates changes in very specific regions causing greater variations in the neutral density structure. Empirical models have greater difficulty representing this more varied structure due to their statistical representation of the neutral atmosphere structure, and errors typically increase to up to 50% (Bowman and Storz, 2003). During these times, the data assimilation system must rely more on improved driver specification to correctly 'drive' the physical model representation.

The most recent work has concentrated on incorporating the high latitude forcing into the data assimilation system. This forcing includes knowledge of the spatial and temporal variations of the convection electric field and the auroral precipitation. Inaccurate knowledge of these drivers in data assimilation systems for space weather applications will lead to limitations in improving the specification further. Compared with the solar wind parameters that force the magnetosphere, the drivers of the upper atmosphere, although well understood, have been to date poorly quantified. This research has sought to better quantify the balance between solar and magnetospheric forcing over the range of solar and geomagnetic activity through the implementation of an ensemble Kalman filter to specify the drivers for the troposphere. Since the solar heating at low latitudes and the magnetospheric sources at high latitudes control the magnitude and spatial distribution of the global circulation, these drivers strongly affect the neutral composition and density structure, and as a result, the ensemble Kalman filter approach for specifying the drivers is suited for the thermosphere. Further, the improved driver specification, in turn, improves the density specification in the data assimilation system.

The Data Assimilation System

Because of its specific design to handle nonlinear systems, an extended form (Costa and Moore, 1991) of the Kalman filter is used. The Kalman filter is an alternative way of implementing the least squares method by sequentially solving the problem with each new observation.

$$y = Hx + \varepsilon$$

where y is the observation, x is the state, and H is the linear relationship between the state and observation. ε represents the error in the observation that is to be eliminated. The primary data assimilation system, based on the extended Kalman filter, can also be written in ensemble form, as will be shown in a moment. The elements of the state vector represent the driver (ap), the density/temperature at each grid point over the globe.

To propagate the estimated state and its error variance-covariance matrix forward in time, CTIM is used.

$$\bar{x} = \Phi_{CTIM} \hat{x}$$

and

$$\bar{P} = \Phi_{CTIM} P \Phi_{CTIM}^{T}$$

where $\hat{x}$ is the previous best estimate, $\bar{x}$ is the model propagated state, P is the error covariance matrix of the previous best estimate of the state, and $\bar{P}$ is the model propagated error covariance matrix. The physical model, CTIM, is used to calculate the state transition matix, Φ_{CTIM}, where the superscript, T, is the transpose.

The weighting, or Kalman gain, K, is determined from the propagated state error covariance matrix, $\bar{P}$, the observation error variance-covariance matrix, R, and the mapping matrix, H, as

$$K = \bar{P}H^{T}\left(H\bar{P}H^{T} + R\right)^{-1}.$$

The calculated Kalman gain then is used to map the observation vector correction to the model propagated state as

$$\hat{x} = \bar{x} + Ky$$

where the new associated error covariance matrix is calculated as

$$P = (I - KH)\bar{P}(I - KH)^{T} + KRK^{T}.$$

The extended Kalman filter equations are then repeated, using the corrected state estimate and its corrected error variance-covariance matrix, to obtain a state and state error variance-covariance matrix for the next observation time.

The advantage of writing the equations of the Kalman filter in extended form comes from the continual correction to the nominal state. Typically, estimation methods specify the deviation from a nominal state. This deviation is assumed linear, which is an adequate assumption if the deviation is sufficiently small enough to lie within the linear regime. If, however, the state is not well know, as can happen during storm conditions, the current state estimate may not lie within this linear regime of the nominal state making the linear assumption invalid. The extended version of the Kalman filter allows for the continual correction to the nominal state, which in turn helps minimize the effects of nonlinearities by continually decreasing the difference between the current and nominal states.

Additional improvements include the ensemble version of the extended Kalman filter (Evensen et al., 2000; Keppenne, 2000; Houtekamer and Mitchell, 1998) which avoids the numerical difficulties of calculating the transition and covariance matrices, allowing one to correlate the drivers with the thermospheric response. The correlation length between adjacent points within the thermosphere is very short, and therefore, adjacent points are poorly correlated in the transition and covariance matrices of the Kalman filter. However, the relationships between driver, density/temperature, and composition change are strongly correlated at a given point and must be properly represented in the transition and covariance matrices. Including these correlated points in the transition matrix makes traditional calculations of the transition and covariance matrices too tedious, even for a computer, and therefore impractical, and an ensemble version of the extended Kalman filter must be applied.

Although 20 members were used in the ensemble Kalman filter in this research, a simplified schematic, using 3 members, is shown in figure 1 to illustrate the mechanics of the ensemble Kalman filter.

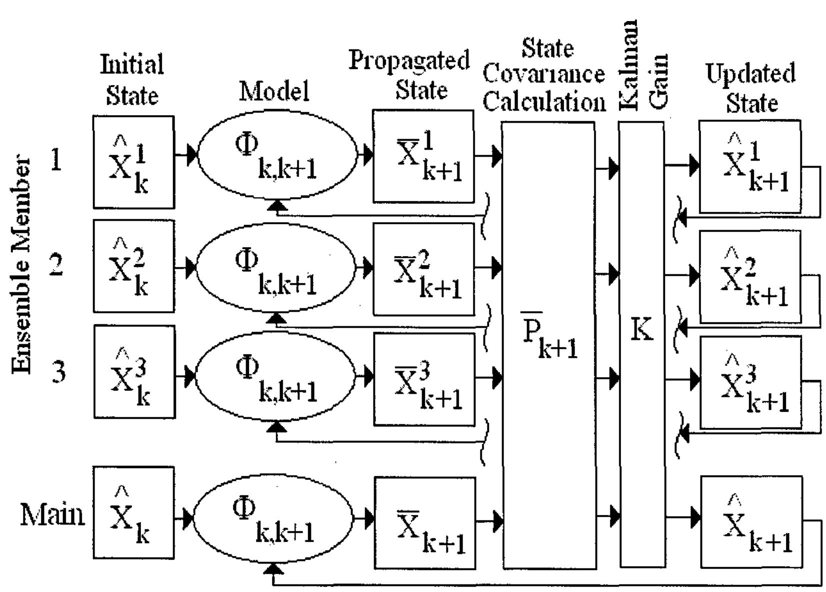

Figure 1: An 3-member ensemble Kalman filter example.

The ensemble Kalman filter uses direct calculation of the covariances based on the Monte Carlo statistics of an ensemble of separate filters. In the ensemble Kalman filter, each member of the ensemble is a separate filter estimating a separate state. The ensemble Kalman filter uses the variance in these separate states to estimate the covariance of the entire ensemble.

A set of 20 filter processes are run in parallel where the initial states are randomized with a Gaussian number generator. The standard deviation of the random number generator is the same as that for the desired a priori state error covariance matrix. As each of these processes of the ensemble is propagated independently forward in time, the resultant distribution of the propagated states of the ensemble will have a new associated error variance-covariance matrix. Thus, the propagated state error covariance matrix, $\overline{P}$, may be calculated directly from the ensemble of propagated states using the standard statistical equations below:

$$\sigma_{ii}^2 = \frac{\sum_{k=1}^{m} \left(\overline{x}_{i,k} - \mu_i\right)^2}{m-1} \tag{1}$$

which provides the diagonal, or variance, elements of $\overline{P}$. The ensemble is made of m members. σ_{ii}^2 is the variance of all of the member states in the ensemble of the ith diagonal element, and μ_i is the mean of the ensemble for the ith state element. $\overline{x}_{i,k}$ is the *i*th element of the *k*th propagated member state element. The off-diagonal, or covariance, terms are found by the similar equation

$$\sigma_{ij}^2 = \frac{\sum_{k}^{m} \left(\overline{x}_{i,k} - \mu_i\right)\left(\overline{x}_{j,k} - \mu_j\right)}{m-1} \tag{2}$$

where σ_{ij}^2 is the *i-j*th element of $\overline{P}$. μ_i is the mean of the ensemble for the *i*th state element, and μ_j is the mean of the *j*th state element. $\overline{x}_{i,k}$ is the *i*th propagated state element of the *k*th member, and $\overline{x}_{j,k}$ is the *j*th propagated state element of the *k*th member.

Each member of the initial estimated state, $\overline{x}_i$, is randomized initially and is propagated using the physical model. Once the state is propagated forward to the next time step, the state error variance-covariance matrix is calculated statistically, as described above in equations (1) and (2). As a result, the transition matrix need not be calculated. Since the ensemble caries the state error information, the current error variance-covariance matrix, *P*, need not be stored in memory. Since the current error covariance matrix *P* is stored in the state ensemble.

The ensemble Kalman filter has an advantage over the traditional Kalman filters in that the state error covariance matrix is calculated directly using equations (1) and (2). Also, by calculating the state error covariance matrix directly from the ensemble distribution, the state error covariance matrix avoids the problem of assymetry.

The Importance of Driver Estimation

Compared with the solar wind parameters that force the magnetosphere, the magnitude and spatial distribution of the upper atmospheric drivers, although well understood, are difficult to quantify. To truly have any effect on reducing the errors during storm conditions, specification of the spatial and temporal variations of the convection electric field and the auroral precipitation is required. Without data assimilation, the globally averaged Joule heating rate at a given time is probably only known within a factor of two. At a given location, this uncertainty can rise to a factor of ten. Therefore, research has concentrated primarily on quantifying the high altitude forcing during geomagnetic storm by using the approach of also observing the response, rather than just the conventional input parameters alone. Since a given response defines the magnitude and spatial distribution of the source, vastly more information is available for specifying the drivers as well as the current upper atmospheric conditions. From observing the thermospheric response, research has focused on determining if it is possible to specify the real-time driver and heating distribution from observations of the upper atmospheric conditions alone. Since the dynamics of the composition structure is strongly directed by the distribution of the Joule heating, observing the change in composition should act as an additional source for the upper atmospheric drivers and subsequently should provide a better specification for the change in density through the physical model.

The energy input, primarily through the Joule heating is typically the most significant driver of the changes in neutral composition during geomagnetic storms. As energy is added to the thermosphere, the temperature increases, and the pressure at specific altitudes changes hydrostatically. In a pressure coordinate system, the mechanism can be illustrated as in Figure 2.

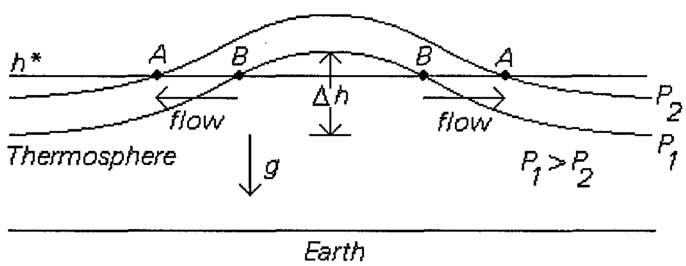

Figure 2. The creation of horizontal winds by increasing the pressure level height.

Localized Joule heating raises the temperature within a given area, and the heights of the pressure levels, say P_1 and P_2, increase at the location where the heating is occurring. In Figure 2, a constant reference altitude, h^*, is chosen so that it passes through the two pressure levels. Because of the localized increase in height of the pressure levels, the pressure is no longer uniform at all locations along h^*, and a pressure gradient results. Since P_1 is at a lower altitude than P_2, by the hydrostatic equation, the pressure at P_1 will be higher, or in other words, the pressure at point B is higher than at point A. As a result of this gradient, a flow occurs from point B toward point A, and thus, a diverging horizontal wind at h^* moves a away in the radial direction from the region of Joule heating.

Since, in pressure coordinates, the atmosphere can be treated as incompressible, the divergence of the flow on the global scale is conserved, a larger circulation pattern is formed and a convergence of the horizontal winds occur at lower altitudes as shown in Figure 3 below.

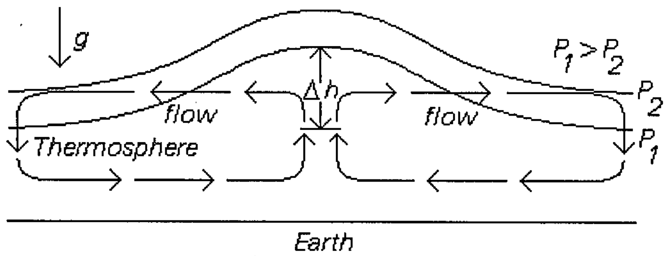

Figure 3: Circulation pattern resulting from the divergence of the horizontal winds at higher altitudes and the balancing convergence at lower altitudes.

The size of the circulation pattern depends largely on the temperature gradient, i.e. the amount of Joule heating and the previous state of the thermosphere. The divergence of the horizontal winds at the higher altitudes is the source of the vertical wind that is responsible for neutral composition changes. The true vertical velocity is a combination of the change in height due to temperature change from the Joule heating and the upward flow resulting from the divergence pattern.

These horizontal and vertical neutral winds are responsible for the transport of the neutral species. The horizontal winds, resulting from the localized Joule heating, transport changes in composition. By observing the neutral composition and density response, the magnitude of the heat sources can be inferred. An example of how this is possible is shown in figure 4. The top panel shows simulated thermospheric density conditions under storm conditions. The middle panel shows typical quiet conditions. Quiet conditions can be estimated with a high degree of accuracy, and any deviation from these conditions are very noticeable and indicate the storm effects. The bottom panel shows the difference between the storm and quiet conditions where the red regions show where the thermosphere is being heated and the density in these regions at a given altitude (450 km) is increasing. Also, in the bottom panel, the electric field patterns are illustrated by the blue outlines. Because the heating (red regions) overlap with the electric field location (blue outlines), a strong correlation between electric field strength and distribution and heating magnitude and distribution can be statistically drawn.

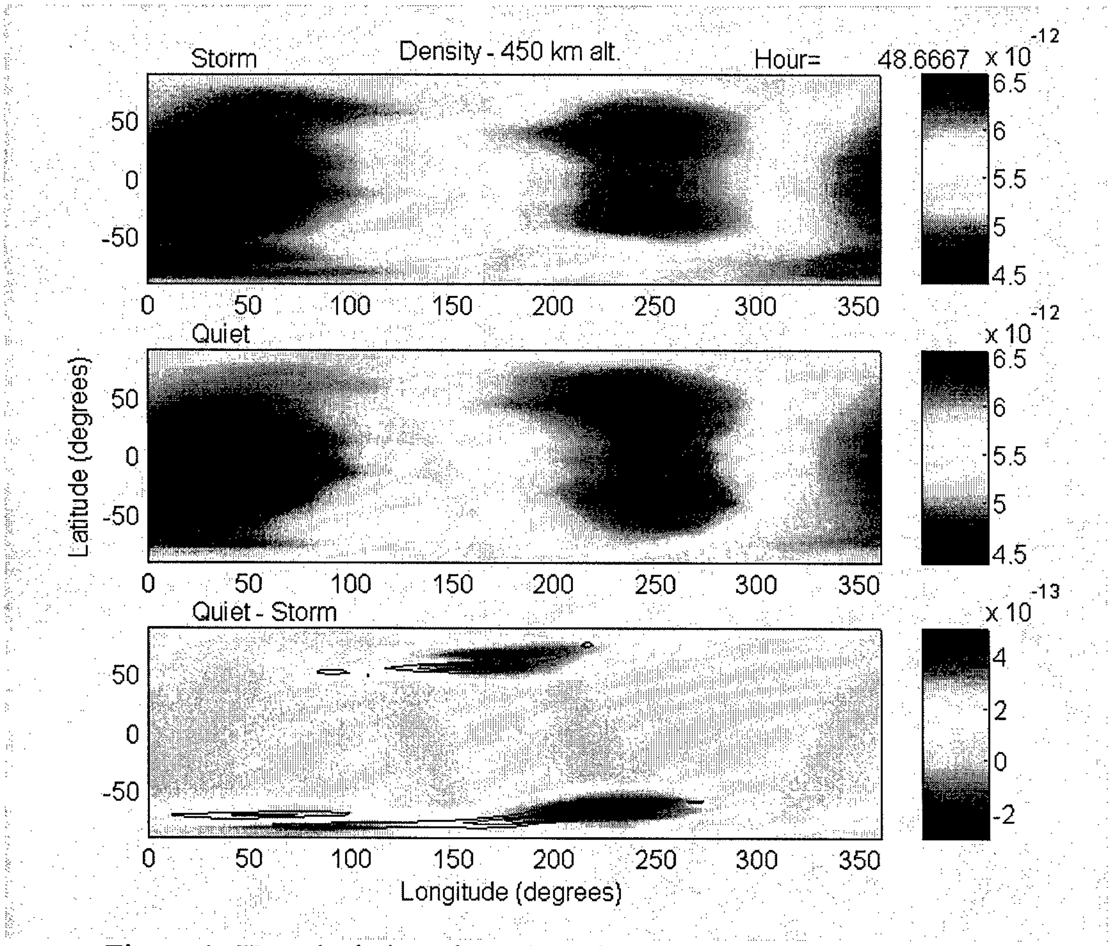

Figure 4. How deviations from the quiet state can indicate the regions of heating due to storm conditions.

Estimating the magnitude and distribution of the drivers enables one to 'drive' the physical model toward the observations. Two examples of controlling the physical model are shown in figures 5 and 6. Figure 5 shows the measurements (indicated with the red triangles) taken by Challenging Minisatellite Payload (CHAMP) during a geomagnetic storm. The storm strength is shown by Ap in the top left corner of each panel. The model output is shown by the blue circles in each panel. Here in figure 4, the model has no driver correction and therefore does not properly represent the storm conditions. As a result of the lack of driver specification, a discrepancy between the model result and CHAMP observation occurs with the resultant percent root mean squared (%RMS) shown in the bottom left side of each panel. Errors range from 31 to 62%, indicating the necessity to include driver specification in the data assimilation system.

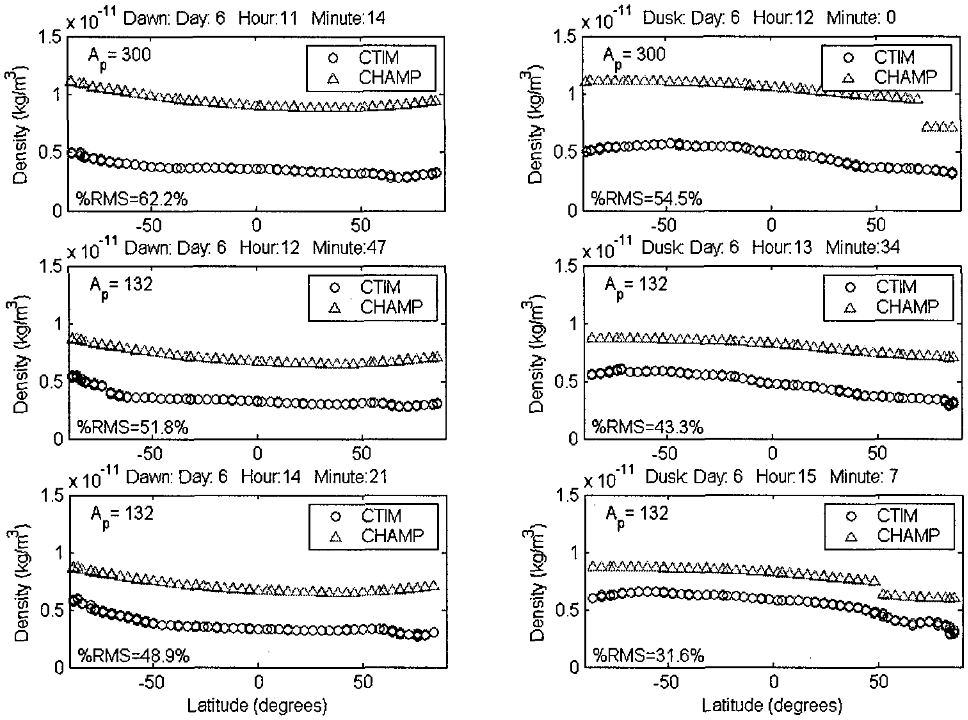

Figure 5: A comparison of CHAMP data and CTIM (without driver specification).

Figure 6 shows a much different story. Here, an attempt is made to estimate the amount of heating in the upper atmosphere. Only the driver is estimated and the physical model is 'driven' based on this estimate. In figure 6, no attempt has been made to correct the other state elements that describe the density; instead, only the driver is corrected and the physical model results are shown.

Specifying the driver alone greatly improves of the physical model prediction, as indicated by the blue circles in figure 6. There is a closer match to the CHAMP measurements (red triangles) as compared to the previous figure 5. Errors range over much smaller values, from 9 to 22%. The values are obtained from specifying the drivers alone. The errors can be further reduced if the density correction is also included. However, figure 6 illustrates the significant influence of driver specification in the accuracy of the data assimilation system.

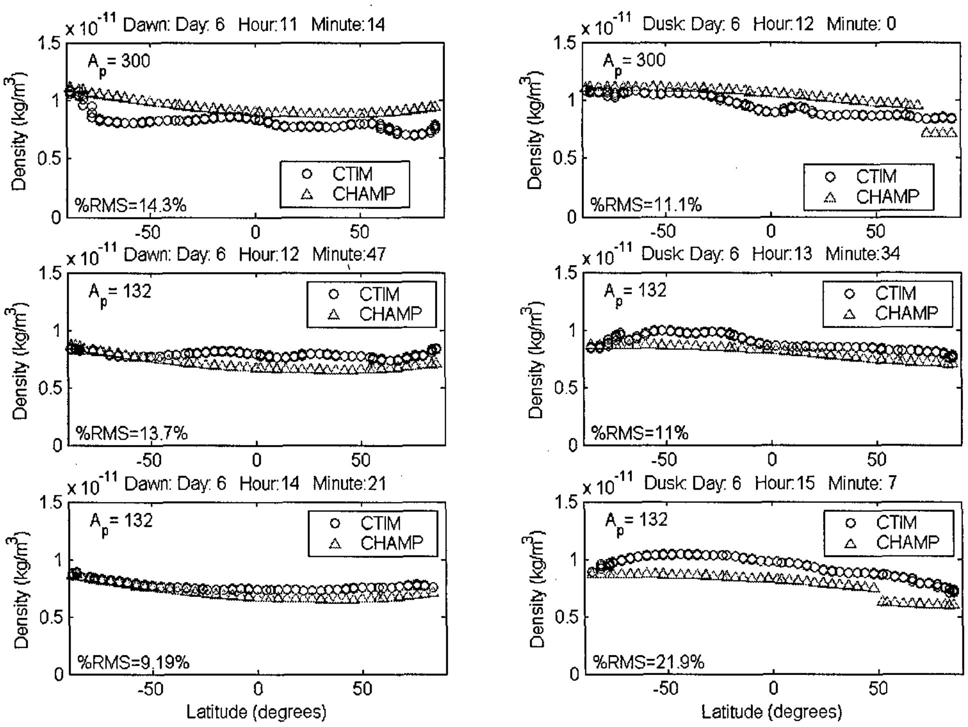

Figure 6: A comparison of CHAMP data and CTIM (without driver specification).

The Capability of the Data Assimilation System

The results in Figure 7 illustrate the simulation of an actual storm during 15-20 April 2001; the power input during this period is shown in the top panel of Figure 7. To stress the system, the truth file is driven by magnetospheric drivers unknown to the Kalman Filter in order to determine the importance of the driver knowledge on the density specification accuracy.

The Kalman filter solution, when the incorrect forcing is applied to the physical model, is illustrated by the red line in the bottom panel of Figure 7. As can be seen, the Kalman filter performs better during the initial quiet conditions, but at the storm onset on April 18, the red line is 'pushed' away from the correct solution since the drivers are incorrectly described. The solution is actually poorer in accuracy during the height of the storm as compared to not using a model at all (yellow line). This result indicates that specifying the drivers and heating distribution is just as important as estimating the final parameters, like the density.

To improve the driver specification, a statistical relationship between the heating and composition change can be described. Through observations of the composition change, the heating distribution is estimated. This estimate is then used to 'drive' the physical model, CTIM, and the results are shown by the blue line in the bottom panel of figure 7.

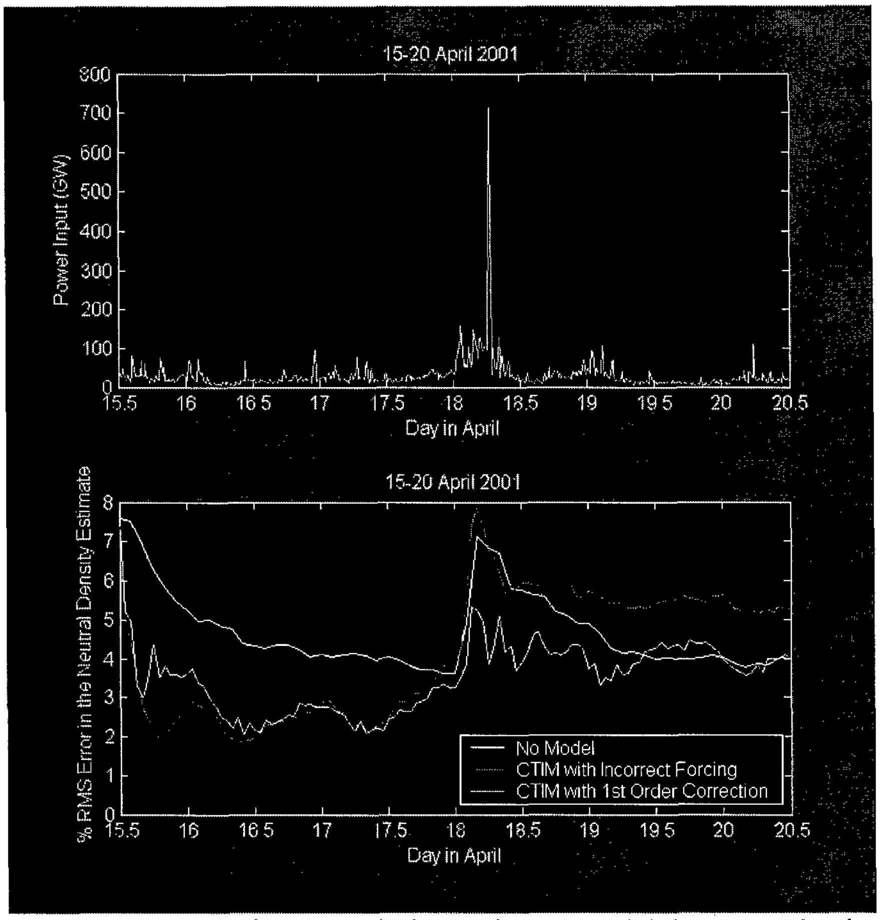

Figure 7: A comparison of solutions with no model, incorrect forcing, and a 1st order correction to the forcing.

Errors that still exist in the density specification can be attributed to errors in the heating distribution knowledge in poorly observed regions. However, estimating the magnitude and the distribution of the heating can reduce errors, particularly during geomagnetic storm conditions.

The errors that still exist come from the nonlinearities between the drivers and the thermospheric response.

General Conclusions

A data assimilation system for specifying the thermospheric density has been built and tested using thermospheric simulation and also data from CHAMP. Results show that quiet geomagnetic conditions can be specified to a high degree of accuracy, but storm conditions pose special problems that have required a closer examination of the thermospheric physics as well as the operation of the filtering techniques. The focus over the most recent years of this project has moved toward specifying the thermospheric forcing since this system is so strongly externally driven. Results have shown that errors during geomagnetic storms can be reduced if the drivers can also be specified. Due to the nonlinear relationship between the drivers and the thermospheric response, special attention will need to be devoted to filtering techniques that are specifically designed for nonlinear systems.

The following publications and conference papers have resulted from this project:

C. F. Minter, T. J. Fuller-Rowell, and M. V. Codrescu, 'The Potential of Remote Sensing for Neutral Atmospheric Density Estimation in a Data Assimilation System', still waiting for review, submitted to *The Journal of the Astronautical Sciences*, February 2005.

T. J. Fuller-Rowell, M. V. Codrescu, C. F. Minter, and D. Strickland, "Application of Thermospheric General Circulation Models for Space Weather Operations", Committee on Space Research Proceedings, accepted, in press, 2005.

C. F. Minter, T. J. Fuller-Rowell, and M. V. Codrescu, 'Specifying the Upper Atmospheric Drivers Using an Ensemble Kalman Filter', American Geophysical Union, Spring Meeting, New Orleans, Louisiana, May 23-27, 2005.

C. F. Minter and T. J. Fuller-Rowell, 'A Robust Algorithm for Solving Unconstrained Two-Point Boundary Value Problems', AAS 05-129, 15^{th} American Astronautical Society/American Institute for Aeronautics and Astronautics Space Flight Mechanics Meeting, Copper Mountain, Colorado, January 23-27, 2005.

C. F. Minter, T. J. Fuller-Rowell, and M. V. Codrescu, 'Upper Atmospheric Driver Determination Using Data Assimilation', National Radio Science Meeting, Boulder, Colorado, January 5–8, 2005.

C. F. Minter, T. J. Fuller-Rowell, and M. V. Codrescu, 'Estimating the Upper Atmospheric Forcing through Observing and Modelling the Thermospheric Response', American Geophysical Union, Fall Meeting, San Francisco, California, December 13-17, 2004.

C. F. Minter, T. J. Fuller-Rowell, and M. V. Codrescu, 'The Challenges of Neutral Atmosphere Data Assimilation', High Altitude Observatory Colloquia, Boulder, Colorado, October 20, 2004.

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C. F. Minter, T. J. Fuller-Rowell, M. V. Codrescu, 'Neutral Atmospheric Density Estimation Using Ridge-Type Estimation Methods', International Union of Geodesy and Geophysics General Assembly in Sapporo, Japan, June 30–July 11, 2003.

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